A Computational Framework for Generating Chemical Profile Inventories and Sustainability Assessment in Process Simulators

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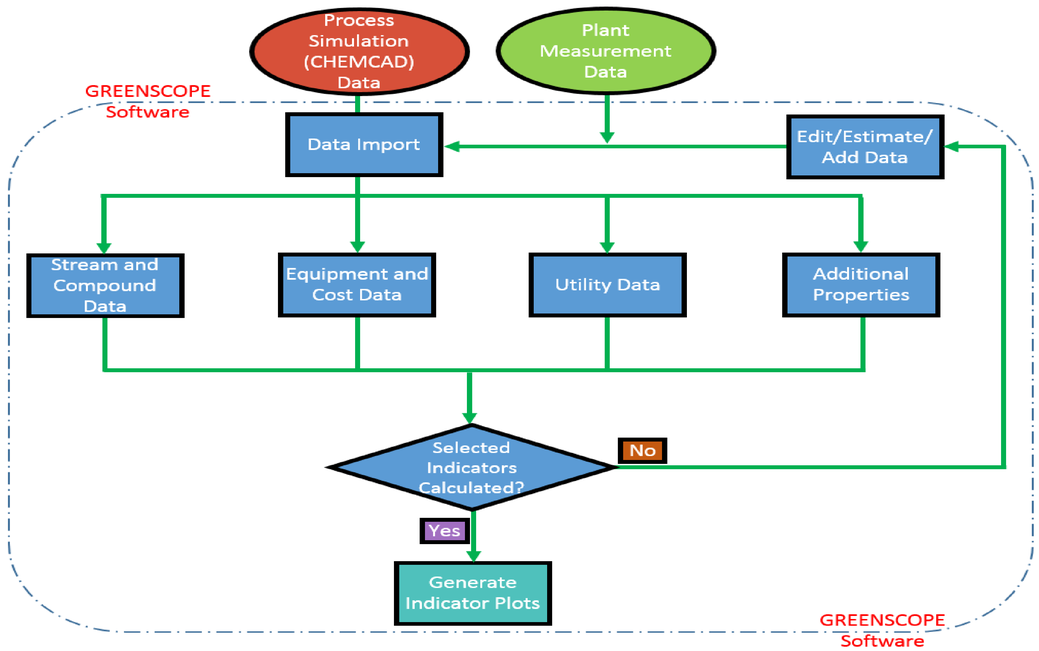
Introduction

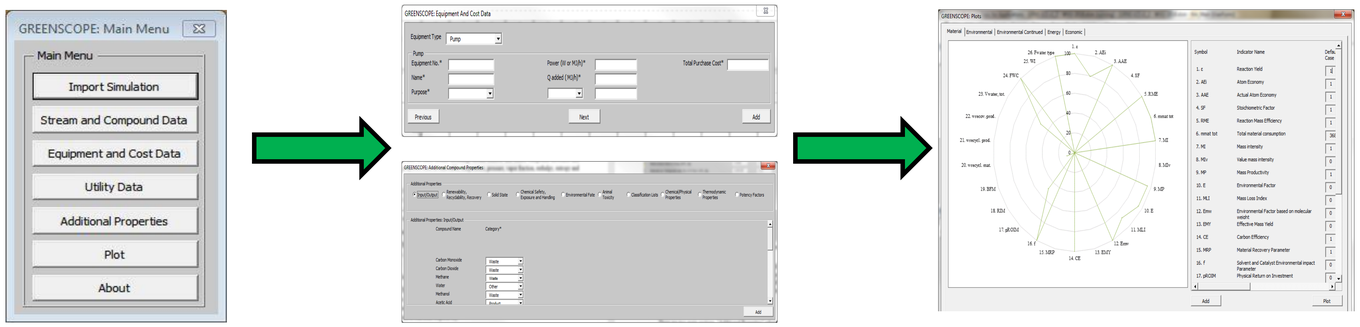
- Process simulators have the ability to represent steady-state and dynamic processes characterized by high-fidelity models.
- However, incorporating life cycle inventory information, consisting of release profiles, resource consumption, for sustainability assessment and decision-making is currently challenging.
- The main challenge is the lack of sustainability analysis features in current process simulation packages.
- This research employs the GREENSCOPE tool Microsoft Excel version, a sustainability assessment tool provided by the U.S. Environmental Protection Agency.
- GREENSCEOPE is enhanced for incorporation into process simulation software.
- This facilitates the generation of life cycle profiles and sustainability assessment of chemical systems.
- The GREENSCOPE tool characterizes overall sustainability performance of a chemical plant in different categories corresponding to material, environmental, energy and economic efficiency indicators.
- An indicator with a value corresponding to the middle of the radar plot represents 0% sustainability for the indicator in question only, and the top edge of the plot corresponds to a value of 100% sustainability for the indicator in question.
- This analysis allows for comparison of candidate designs and operation plans with indicators as a measure for optimum design choice.

Overview of Improved GREENSCOPE Framework



- The improved GREENSCOPE encapsulates the previous version of GREENSCOPE with an automatic data transfer connection.
- The data transfer connection has been applied to CHEMCAD process simulation software (although this can be extended to others).
- GREENSCOPE retains the option for manual entry to edit imported data or add new fields to previously imported data.
- It allows the use of built in databases to retrieve common properties of respective compounds.
- Custom plots may be generated to include the analysis of any combination of material, energy, environmental and economic efficiency through the use of any number of the 139 indicators available in GREENSCOPE.

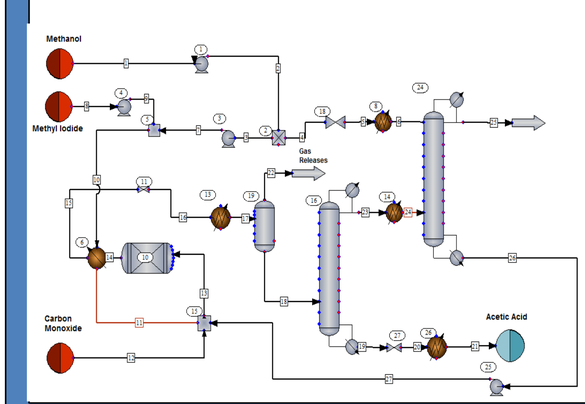
GREENSCOPE Improved Interfaces



Brief Summary of GREENSCOPE Interface

- New interface shows the import feature included in GREENSCOPE to allow for automatic data transfer for analysis.
- Editing or adding data can be performed under the following tabs “Stream and Compound Data” , “Equipment and Cost Data” , “Utility Data” and “Additional Properties.”
- Required data in these software windows are marked with an asterisk and may be either imported automatically or manually entered.
- The window for “Equipment and Cost Data” includes standard equipment such as pumps, reactors and heat exchangers in addition to custom equipment as shown above.
- The window for “Additional Compound Properties” contains several fields pertaining to chemical, physical and thermodynamic properties, chemical exposure and renewability/recyclability/recovery etc. as depicted above.

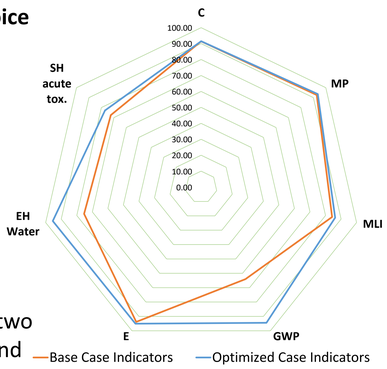
Application of GREENSCOPE : Acetic Acid Simulation in CHEMCAD



Main Factors Considered In Indicator Choice

Potential for global warming
Presence of hazardous materials
Unconverted reactants in waste streams
Waste and greenhouse gases in waste streams.

By selecting the same set of indicators for two cases, GREENSCOPE enables comparison and analysis of these cases.



Conclusions

- For the improved interface between GREENSCOPE and CHEMCAD, the requirements for each category have been streamlined with similar parameters with dependencies grouped together.
- In addition, built-in values from the GREENSCOPE database are automatically updated on the interface.
- New plotting capabilities are introduced in which results are shown on plots under their respective categories, in addition, multiple indicators may be combined for analysis across categories.
- A seamless transfer of data from process simulation software such as CHEMCAD to allow for automatic data transfer has been implemented

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- *Disclaimer*: The views expressed in this (article) are those of the authors and do not necessarily represent the views or policies of the U.S. Environmental Protection Agency.